Equilibrium and Nonequilibrium Responses of Anisotropic XY Ferromagnets

Synopsis of the PhD Thesis

submitted by

Olivia Mallick

Registration No. R-21RS209210330

E-mail:mallickolivia0@gmail.com

Under the guidance of

Prof. Muktish Acharyya

Department of Physics

Presidency University

86/1 College Street, Kolkata-700073, INDIA

1 Introduction:

In the realm of statistical physics, the study of classical XY ferromagnets has long been a cornerstone due to their intriguing properties and phase transitions. The presence of SO(2) symmetry in these systems gives rise to the celebrated Kosterlitz-Thouless (KT) transition in two dimensions [1],[2] where vortices-antivortices play a pivotal role in the phase transition mechanism. The landscape becomes fascinating due to the unconventional phase transitions, characterized by a lack of long-range ferromagnetic order in two dimensions. The higher dimensions introduces new dynamics, where isotropic XY ferromagnets exhibit phase transitions with long-range order, classified within a distinct universality class [3],[4]. Anisotropy plays a crucial role in magnetic model systems. In the case of XY ferromagnets, anisotropy destroys the inherent SO(2) symmetry. Anisotropy manifests in various forms, including bilinear exchange and single-site anisotropy, fundamentally altering the phase behaviour and critical phenomena observed. Bilinear exchange anisotropy refers to the preference for interactions between neighbouring components of the magnetic moments along specific directions, whereas single-site anisotropy signifies the tendency for individual magnetic moments to prefer a particular axis to minimize the energy. Moreover, the effects of disorder further complicate the picture, introducing randomness into the system. The role of such quenched disorder in the thermodynamic phase transition of continuous symmetric magnetic models is a fascinating field of research in statistical and condensed matter physics. Random anisotropy, non-magnetic impurities, and random fields all contribute to the complexity of the phase diagram, influencing the emergence of novel phases and critical behaviours. Equilibrium responses elucidate the stable configuration and properties of these systems at thermal equilibrium, phase transitions and critical phenomena. Beyond equilibrium dynamics, the exploration of non-equilibrium phase transitions in the XY model opens up a new frontier in understanding complex systems. The non-equilibrium responses probe the dynamic evolution of the magnetic systems under external perturbations, systems far from equilibrium, shedding light on phenomena like hysteresis,

relaxation and out-of-equilibrium phase transitions.

In this synopsis of Phd thesis, I embark on a comprehensive investigation into the interplay between anisotropy, disorder, and non-equilibrium dynamics in classical XY ferromagnets[5]. Through statistical analysis and numerical simulations namely Monte Carlo simulation, I aim to elucidate the effect of disorder in the thermodynamic phase transitions (in equilibrium) in these systems, ultimately contributing to a deeper understanding of complex condensed matter phenomena. I have also studied the nonequilibrium phase transition in driven anisotropic XY ferromagnet showing nonequilibrium tricritical behaviours.

2 Outline of my research

2.1 Anisotropic XY Ferromagnet

The Hamiltonian of anisotropic XY ferromagnet reads as,

$$H = -J \sum_{<i,j>} [(1+\Omega) {S_i}^x {S_j}^x + (1-\Omega) {S_i}^y {S_j}^y] \tag{1}$$

for bilinear exchange anisotropy (Ω) and

$$H = -J \sum_{<i,j>} [{S_i}^x {S_j}^x + {S_i}^y {S_j}^y] - D \sum_i [({S_i}^x)^2 - ({S_i}^y)^2] \tag{2}$$

for single-site anisotropy (D).

where ${S_i}^x (= \cos\theta_i)$ and ${S_i}^y (= \sin\theta_i)$ correspond to the components of the two-dimensional spin vector (at i-th lattice site) having unit length $|\vec{S_i}| = 1$. θ is the angle (measured with respect to the positive X axis) of the spin vector. It may be considered a rotor at each lattice site, which can point in any direction in two dimensional XY plane. $J(> 0)$ is the nearest neighbour ferromagnetic interaction strength. Physically the bilinear exchange anisotropy (Ω) brings the non-uniformitity in the effective strengths of rel-

ative ferromagnetic interactions for x and y components of the spin vector. The single-site anisotropy (D)[6] represents the effective and intrinsic crystal field.

2.2 Numerical approach

Monte Carlo simulations are employed to study the system. A cubic lattice of $L \times L \times L$ is considered where the spin vectors in each lattice site are represented by $\theta(x, y, z) \in (0, 2\pi)$. Periodic boundary conditions are imposed in all three directions. The system starts in a high-temperature paramagnetic phase with random initial spin orientations, i.e.$< \vec{S_i} >= 0$. At a given temperature T (in units of J/k_B where k_B is the Boltzman constant) a lattice site with initial configuration $\theta_i(x, y, z)$ is randomly selected among the L^3 options. A new configuration $\theta_f(x, y, z)$ is randomly chosen. The acceptance probability P_f of the new configuration is determined using Metropolis single spin-flip formula, P_f =Min[exp $(-\frac{\delta H}{k_B T})$] ($\delta H$ is change in energy results from change in configuration) [7],[8]. L^3 number of such random update is defined as one Monte Carlo Step per Site (MCSS). Note that it is the unit of time in the simulation. The simulation runs for t MCSS, discarding the initial t' transient steps to allow the system to reach equilibrium. Thermodynamic quantities are calculated by averaging over the remaining $t-t'$ MCSS, assuming ergodicity, meaning the time average represents the ensemble average.

Using the above scheme I have simulated the three-dimensional anisotropic XY model in different disorder environments. In order to determine the critical behaviour in equilibrium phase transitions the main quantity of interest is magnetization. The instantaneous components of magnetisations at any i-th lattice site are

$$m_x = \frac{1}{L^3} \sum_i S_i^x = \frac{1}{L^3} \sum_i \cos(\theta_i)$$

and

$$m_y = \frac{1}{L^3} \sum_i S_i^y = \frac{1}{L^3} \sum_i \sin(\theta_i).$$

The instantaneous equilibrium magnetisation is measured as

$$m = \sqrt{m_x^2 + m_y^2}.$$

The average (over time) magnetisation $M =< m >$. The susceptibility is determined by

$$\chi = \frac{L^3}{k_B T}(< m^2 > - < m >^2).$$

The specific heat is measured as

$$C = \frac{L^3}{k_B T^2}(< E^2 > - < E >^2),$$

where E is the energy density, calculated from the Hamiltonian.

To characterize and quantify the phase transition in the thermodynamic limit using finite size scaling analysis, I also have measured the fourth-order Binder cumulant.

$$U_L = 1 - \frac{< m^4 >}{3< m^2 >^2}$$

This has been utilised to determine the critical exponents and universality classes.

2.3 Phase transition in Anisotropic XY ferromagnet with Random Anisotropy

The magnetic anisotropy plays a crucial role in determining the critical behaviour of magnetic model systems. The isotropic XY classical ferromagnet possesses SO(2) symmetry, which is responsible for the appearance of vortex-antivortex pairing and lack of long-range ferromagnetic ordering in two dimensions. There is no conventional phase transition present associated with symmetry breaking. This is what makes them peculiar from other phase transitions known as Kosterlitz-Thouless phase transitions. The anisotropy breaks the SO(2) symmetry in XY ferromagnet. This broken SO(2) symmetry would lead to the destruction of vortex (and antivortex) with the

appearance of long-range ferromagnetic ordering in the system. The three-dimensional anisotropic XY ferromagnet is studied by extensive Monte Carlo simulation with the Metropolis single spin flip algorithm. I report the results of constant anisotropy and variable anisotropy (having specific statistical distributions), the phase boundaries and the corresponding critical exponents[9] in the ***Chapter 2*** of the thesis.

First, anisotropy is considered constant for all spin-spin interactions. The system is gradually cooled down from a high-temperature paramagnetic state. As the temperature decrease magnetization grows continuously and eventually saturates to unity. The corresponding susceptibility exhibits a peak at specific temperature. From the position of the peak of susceptibility the pseudocritical temperature (the critical temperature for finite-sized system) is obtained. The peak of susceptibility reflects the existence of conventional para-ferro phase transition for three dimensional anisotropic XY ferromagnet [Figure-1 & 2 of [9]].

For constant anisotropy, the ferro-para phase transition occurred at higher temperatures compared to isotropic systems. Figure-1 shows the pseudocritical transition temperature as function of the strength of constant anisotropy. The transition temperature increases linearly with the strength of anisotropy. The straight line fit estimates the pseudo-critical temperature $T_c = 2.33J/k_B$ for $\Omega = 0$. This is in good agreement with MC estimate of T_c for isotropic XY ferromagnet in three dimensions [3]. Moreover for $\Omega = 1$, the system maps to XX model. The pseudocritical temperature for $\Omega = 1$ is closer to that for the MC estimate ($T_c = 4.511$) of 3D Ising ferromagnet. This linear increase can be qualitatively explained by the enhanced ordering bias introduced by anisotropy, which requires more thermal energy to disrupt, thereby raising the pseudo-critical temperature.

However, a completely different scenario emerged when anisotropy is random but statistically distributed. The randomness is introduced by statistically distributing the anisotropy over the space using uniform, Gaussian, and bimodal distributions, ensuring that the mean strength of the anisotropy all over the space is zero($< \Omega_{ij} = 0 >$). The growth of magnetic order by cooling the system from a high temperature disordered phase is studied. For all three

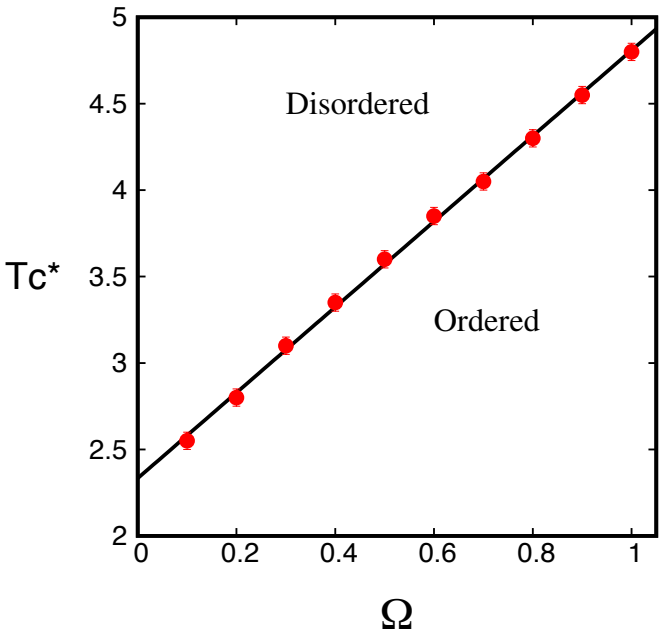

Figure 1: The pseudocritical temperature (T_c^*) is plotted against the strength of the constant anisotropy (Ω). The fitted straight line is $T_c^* = a\Omega + b$ where $a = 2.4757 \pm 0.0289$ and $b = 2.3333 \pm 0.0179$ [9].

distributions, the system is found to order ferromagnetically at lower temperatures as the width (and standard deviation) of the distribution is increased. The pseudocritical temperature decreases as the width of the distribution increases. Figure-2 shows the phase boundaries for different distributions of anisotropy in ($\sigma - T_c^*$) plane. This is due to the fact that, in case of distributed anisotropy, the different spin-spin interactions experience different values of the strength of the anisotropy.As a result, the system cannot be biased in the form of ordering. Hence, the distributed anisotropy plays the role of a disordering field and causes the reduction of pseudocritical temperatures. It may be noted here that for vanishingly small standard deviation ($\sigma \to 0$) of the distributed anisotropy, the pseudocritical temperatures become insensitive to the nature of the distribution and approach the critical value of that of the isotropic XY ferromagnet in 3D.

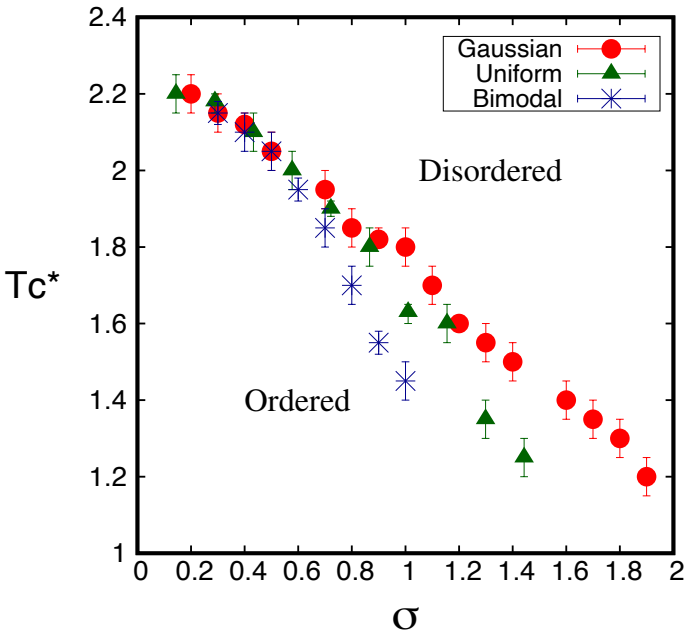

Figure 2: The pseudocritical temperature (T_c^*) is plotted against the standard deviation (σ) of the different distribution of the random anisotropy (Ω_{ij}). The errorbars are the maximum temperature range arising from the stepsize of cooling the system [9].

A dedicated finite-size scaling analysis concretes the evidence in favour of conventional ferro-para phase transitions in an anisotropic XY system in the thermodynamic limit. The fourth-order Binder cumulant estimates the critical temperatures in the thermodynamic limit [Figure-5 of [9]]. When the system size increases, a divergent property emerges in the susceptibility curve at the phase transition point which indicates a second-order phase transition. The critical exponents for the scaling laws ($M \sim L^{-\frac{\beta}{\nu}}$ and $\chi \sim L^{\frac{\gamma}{\nu}}$) are calculated. The findings indicate that anisotropic XY ferromagnets belong to a different universality class than isotropic XY ferromagnets. Moreover, the presence of random anisotropy shifts the system into yet another distinct universality class, highlighting the profound influence of anisotropy on the critical behaviour and universality of these systems.

2.4 Effects of Non-magnetic Impurity

The introduction of non-magnetic impurities in anisotropic XY ferromagnets significantly influences their critical behaviour and phase transitions. These impurities disrupt the magnetic ordering, lowering the critical temperature and altering the universality class, thereby providing insights into the complex interplay between disorder and anisotropy in magnetic systems. In the ***Chapter 3*** of my thesis, I have discussed the effects of non-magnetic impurity on the critical phenomena of anisotropic XY ferromagnet in three dimensions. Two different types of anisotropy, namely the bilinear exchange type and single-site anisotropy are considered here. The thermodynamic variation of magnetisation (M), susceptibility (χ) and the specific heat (C) have been studied systematically through extensive Monte Carlo simulations [10]. The non-magnetic impurity is implemented in the anisotropic model by considering simply few sites (randomly chosen with probability p) having $\vec{S} = 0$. This non-magnetic impurity (p) acts as quenched disorder in the system.While cooling the system for a fixed set of values of the strength of bilinear exchange anisotropy (Ω) and the concentration of impurity (p), it is observed that the order parameter or the magnetisation (M) transits from zero to non-zero value continuously, indicating a continuous phase transition. The susceptibility (χ) and specific heat (C) exhibit maxima at specific temperature. The pseudocritical temperature ($T_c{}^*$) is determined from the temperature at which the susceptibility (χ) attains its maximum value.

The pseudocritical temperature has been observed to depend on the strength of anisotropy (Ω) and concentration of impurity (p). Figure-3 shows the variation of $T_c{}^*$ as function of Ω for four different values of p. For any fixed value of p, the pseudocritical temperature increases as the strength of anisotropy (Ω) increases. The increase in impurity concentration lowers the transition temperature at constant strength of anisotropy. It should be noted here that the critical temperature is also found to decrease with increasing impurity concentration for isotropic XY ferromagnet in three dimensions [5].

In the second part of this work, the effect of non-magnetic impurity on the single-site anisotropic XY ferromagnet is studied. As the system is cooled

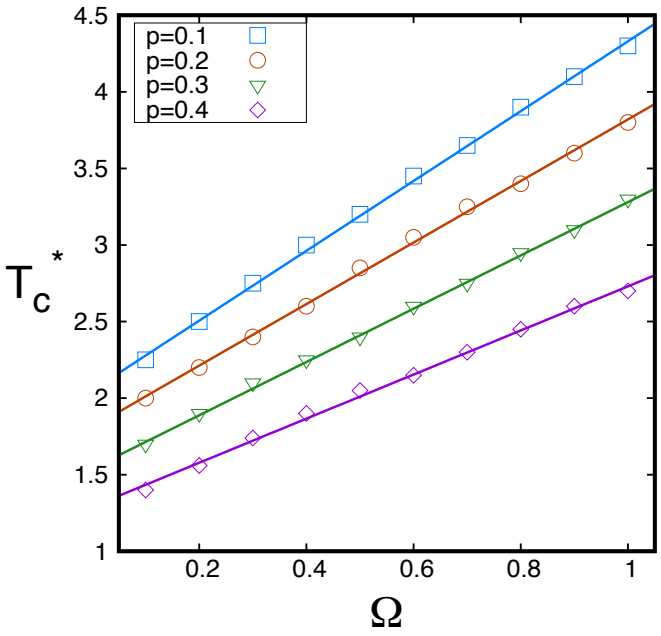

Figure 3: The pseudocritical temperature (T_c^*) is shown as a function of the strengths of the bilinear exchange type of anisotropy (Ω) for different impurity concentrations (p). The solid lines represent corresponding linear best fit $T_c{}^* = a + b\Omega$ [10].

with small temperature steps, at fixed value of single-site anisotropy (D) and fixed impurity concentration (p), the magnetization (M) gradually grows from zero to non-zero value, indicating a continuous phase transition.

The susceptibility (χ) and specific heat (C) peak at a certain temperature marking the point of phase transition. Figure-4 shows the variation of $T_c{}^*$ as a function of impurity concentration (p) for four different D. The pseudo-critical temperature falls linearly with p. It is pertinent to note that the pseudocritical temperature ($T_c{}^*$) increases with D for the fixed value of impurity concentration p.

The impurity in the system acts as quenched random disorder and reduces the critical temperature for both types of anisotropy. Conversely, the anisotropy (both types) destroys the inherent SO(2) symmetry of XY fer-

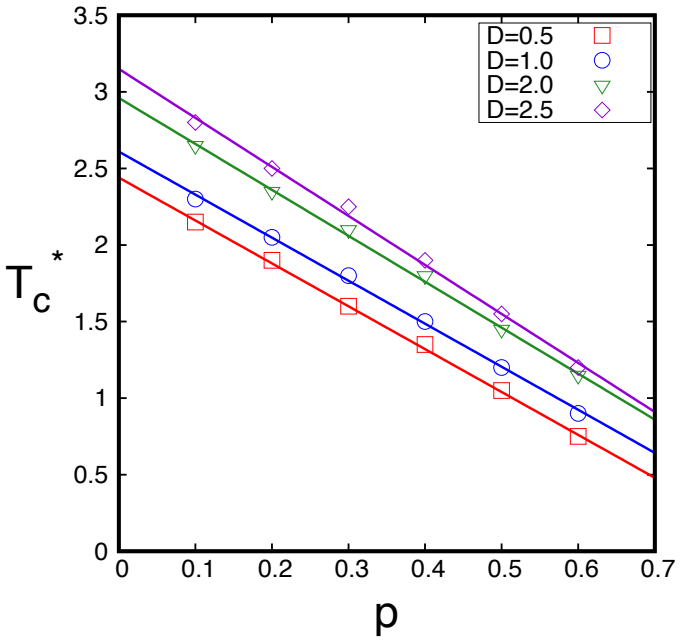

Figure 4: The pseudocritical temperature (T_c^*) is shown as a function of impurity concentration (p) for different strengths of anisotropy (D). The solid lines represent corresponding linear best fits $T_c^* = a - bp$ [10].

romagnet and offers the system to be ordered ferromagnetically at higher temperature regime.

2.5 Critical behaviour of anisotropic XY ferromagnet in presence of quenched random field

In ***Chapter 4***, I have discussed the effects of quenched randomness in form of random fields. The lower critical dimension for the quasi-long-range ordered phase is 3.9 (obtained from a functional renormalization group study) [11],[12]. No ordering occurs for d=2,3 RFXYM. The domain growth and aging in the random field XY model in 2 and 3 dimensions are studied by using Large-scale Monte Carlo simulations [13]. The anisotropy offers a di-

rectional preference and destroys the inherent SO(2) symmetry. It would not be surprising to expect the order-disorder transition in three-dimensional XY model, in the presence of a random magnetic field. The random magnetic field would play the role of random disorder which may lead to the occurrence of long-range order and the ferro-para phase transition in anisotropic XY model in three dimensions [14].

The Hamiltonian of such system in the presence of random field is represented by,

$$H = -J \sum_{<i,j>} [(1+\Omega) S_i{}^x S_j{}^x + (1-\Omega) S_i{}^y S_j{}^y] - \sum_i \vec{h_i} \cdot \vec{S_i} \qquad (3)$$

The random field $\vec{h_i} = (h\cos\phi_i, h\sin\phi_i)$ in each lattice site represents the quenched disorder, described by field strength $h = |\vec{h_i}|$ and angle variable ϕ_i. The randomness of the field is governed by the random directions only (magnitude of field h is constant). The average (over the lattice) value of random field is zero ($< h_i >= 0$).

First, a random field of fixed magnitude (h) is considered but the direction (angle ϕ_i) is distributed uniformly between 0 to 2π. This is labeled as 'A-type' random field. The random field having a null gross effect ($< \vec{h_i} >= 0$) may strongly govern the critical behaviour of anisotropic XY ferromagnet. As the system is gradually cooled down from a high-temperature disordered phase, the spins get ordered. Magnetization grows continuously from zero to non-zero value. The corresponding susceptibility exhibit maxima at certain temperature. The results indicate the presence of long-range order and phase transition from a paramagnetic to a ferromagnetic state. The pseudo-critical temperature of the phase transition is obtained from the position of the peak of the susceptibility.The pseudocritical temperature decreases as the strength of the random field is increased. On contrary the constant anisotropy imposes a directional preferences on the spins, increases the critical temperature of the system[9]. The random field decreases critical temperature by introducing a disorder into the system. The system gets ordered at lowered temperature. The less amount of thermal energy required to transit into disorderd state. The reduction of the pseudocritical temperature is depicted in Figure-5 for

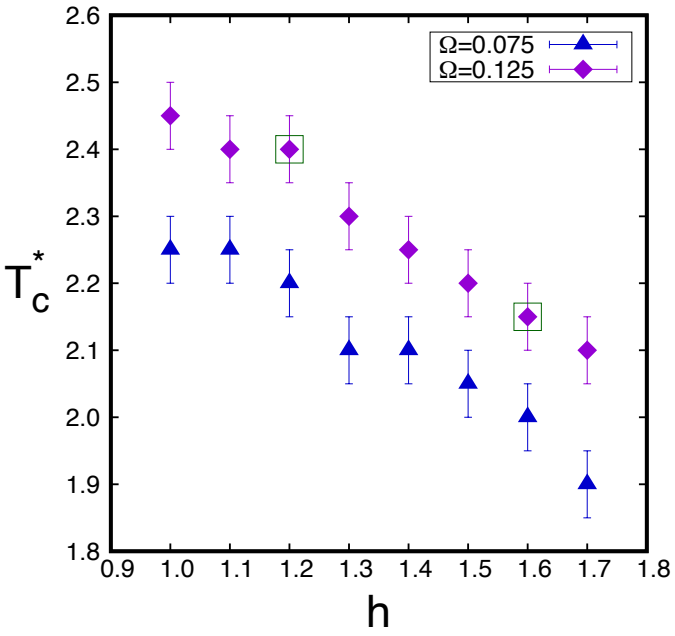

Figure 5: The pseudocritical temperature (T_c^*) (obtained from the peak position of susceptibility) plotte as a function of random (with full circular symmetry) field stregth (h) for different values of anisotropy (Ω). The error-bars are the maximum temperature range arising from the stepsize of cooling the system [14].

two different values of the strengths of the anisotropy. Certainly, the upper points at each field strengths corresponds to the higher anisotropy strength.

So, it offers a competition between constant anisotropy and the random field in the context of having critical temperatures. Former promotes the spin alignments in its favour and increases critical temperature, the later introduces disorder into the system and reduces critical temperature. An interesting question arises in that context. Can the random field nullify the effect of anisotropy? Precisely, is it possible to have the critical temperature for three-dimensional isotropic XY ferromagnet by tuning the values of the strengths of the random field and that of the constant anisotropy?

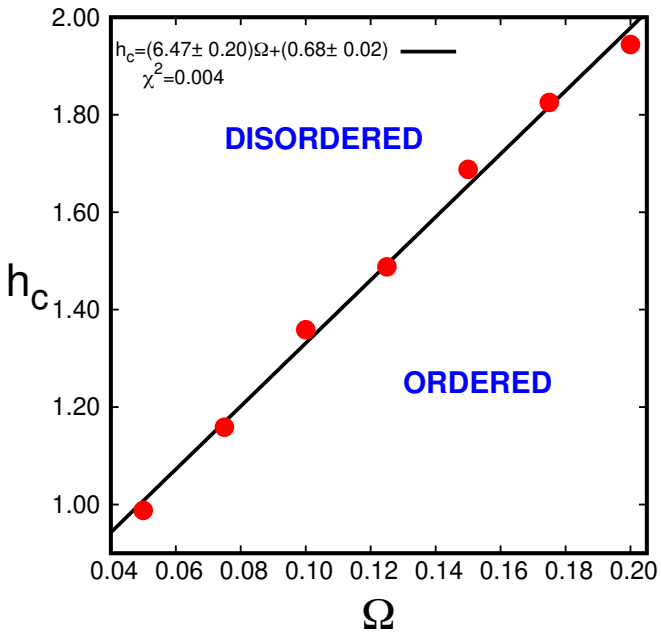

Figure 6: The compensating field (h_c) is plotted as function of anisotropy strength (Ω). The compensating field has been calculated from the linear interpolation around the true critical temperature ($T_c = 2.206$) of the isotropic XY system. The data points are fitted with a straight line. The regions of ordered and disordered phases are separated by this line [14].

The strength (depending on the strength of anisotropy) of the random field required to get the value of critical temperature for three dimensional isotropic XY ferromagnet may be called the compensating field (h_c). The compensating field (h_c) needed to achieve the critical temperature $T_c = 2.206$ [3] for three-dimensional isotropic XY ferromagnet are obtained for different strengths of anisotropy. The pairs of (Ω,h_c) are plotted in Figure-6 and fitted to a straight line. The region below this line exhibits a ferromagnetically ordered phase while the region above corresponds to a disordered phase. The finite size scaling analysis validates the order-disorder transition in the presence of random field and growth of critical correlation in thermodynamic limit.

Then I have studied critical behaviours of the anisotropic XY ferromagnet (in three dimensions) the random field is circumscribed about an angular window. This is labeled as 'B-type' random field. Here also the average field $< \vec{h_i} >= 0$. The pseudo-critical temperature as a function of $\delta\phi$ (keeping the magnitude of field strength) fixed for three different anisotropy strength shown in Figure-7. As the random field angle (ϕ) constricts from circular symmetry ($4\delta\phi = 2\pi$) to the angular window, the pseudo-critical temperature begins to elevate monotonically.

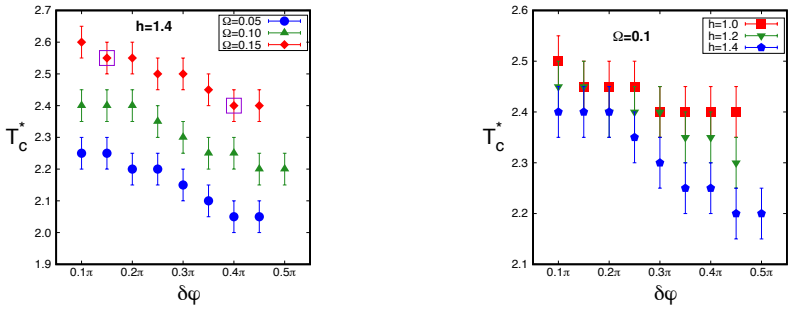

Figure 7: (a)The variation of the pseudocritical temperature ($T_c{}^*$) with the angular extension ($\delta\Phi$) of the random field with tmagnitude $h = 1.4$ for three different strengths of the anisotropy (Ω). (b) The variation of the pseudocritical temperature ($T_c{}^*$) with the angular extension ($\delta\Phi$)at constant anisotropy $\Omega = 0.1$ for three different strengths of the random field. The errorbars are the maximum range arises from the stepsize of cooling the system [14].

For fixed strength of anisotropy, the variation of the pseudo-critical temperature ($T_c{}^*$) has been studied as a function of the angular extension for three different magnitudes of 'B-type' random fields. The results are shown in Figure-7. For stronger magnitude of random field, the pseudo-critical temperature ($T_c{}^*$) has been found to decrease with increasing angular extension ($\delta\phi$).

2.6 Non-equilibrium phase transition and tricritical behaviour of anisotropic XY ferromagnet

Non-equilibrium phase transitions occur in systems driven by external forces or subjected to time-dependent perturbations. These transitions often exhibit novel and intriguing phenomena due to the interplay between the perturbing field and the intrinsic relaxation time of the system. In continuous symmetric magnetic models, the spin vectors describe alignments of the magnetic moments in the system which can exhibit spontaneous symmetry breaking when temperature or other control parameters cross a critical value. In this context, investigating the breaking of dynamical symmetry in continuous symmetric models during non-equilibrium ferromagnetic phase transition is of particular interest.The anisotropic XY ferromagnet driven by a sinusoidally oscillating magnetic field has been analyzed [15] and found to have a dynamic phase transition depending on the frequency and amplitude of the driving magnetic field. Multiple non-equilibrium phase transitions have been observed[16] in the three-dimensional anisotropic Heisenberg ferromagnet driven by elliptically polarized time-dependent (with no space dependence at any instant of time) magnetic field. The phase transition may be discontinuous (first order) or continuous (second order). However, the scenario where both types of phase transitions occur is certainly interesting. This behaviour is known as tricritical behaviour. This question has been addressed in the present study through a detailed Monte Carlo investigation [17]. All the results of the investigation of nonequilibrium behaviour are given in ***Chapter 5*** on my thesis.

The Hamiltonian of such an anisotropic (both bilinear exchange type as well as single-site anisotropy) XY ferromagnet irradiated by an elliptically polarized propagating magnetic field wave is given by the following equation.

$$H(t) = -J \sum_{i,j} [(1+\Omega) {S_i}^x {S_j}^x + (1-\Omega) {S_i}^y {S_j}^y] - \sum_i \vec{h_i(t)} \cdot \vec{S_i} \qquad (4)$$

for bilinear exchange anisotropy (Ω) and

$$H(t) = -J \sum_{i,j} [{S_i}^x {S_j}^x + {S_i}^y {S_j}^y] - D \sum [({S_i}^x)^2 - ({S_i}^y)^2] - \sum_i \vec{h_i}(t) \cdot \vec{S_i} \quad (5)$$

for single-site anisotropy (D).

The term $\vec{h_i}(t) \cdot \vec{S_i}$ corresponds to the Zeeman term or spin-field interaction term. The spatiotemporal variations of the elliptically polarized magnetic field wave the following mathematical form $\vec{h}(t) = \hat{x}h_x + \hat{y}h_y = h_{0x} \cos(2\pi ft - \frac{2\pi}{\lambda}z)\hat{x} + h_{0y} \sin(2\pi ft - \frac{2\pi}{\lambda}z)\hat{y}$, where f and λ represents the frequency and wavelength of the field wave. The field is propagating along the z direction.

In the high-temperature random phase, the order parameter is zero ($\vec{Q} = Q_x\hat{x} + Q_y\hat{y} = 0$). As the system is getting gradually cooled, the order parameter component Q_x acquires a non-zero value where the y component remains zero ($Q_y = 0$). Below a certain pseudo-critical temperature (or dynamic transition temperature), the system is found to get dynamically ordered ($Q_x \neq 0$) for the x-component of dynamic order parameter. This dynamic phase transition is accompanied by *partial* breaking of the dynamical symmetry of the order parameter $\vec{Q}$.

The dynamic transition temperature is found to vary with the field amplitude (h_{0x}, where the y component h_{0y} is kept fixed) of the elliptically polarized propagating magnetic field wave and the strength of bilinear exchange anisotropy (Ω). The transition temperature increases as the strength of anisotropy increases for constant field amplitudes. On the other hand, the system is found to achieve a dynamic ordered phase at a lower transition temperature as the field amplitude (h_{0x} only) increases for constant strength of anisotropy.

Figure-8 shows the comprehensive phase diagram (the image plot of the transition temperature), of such a non-equilibrium phase transition, in a plane described by $r = \frac{1-\Omega}{1+\Omega}$ and $p = \frac{h_{0x}}{h_{0y}}$. When constructing the phase diagrams, all pseudo-critical temperatures (transition temperature for finite-sized system) are calculated from the peak position of the thermal variation of $Var(Q_x)$. This is basically a surface, below which the system is in ferromag-

netically ordered phase and above which the disordered phase is obtained.

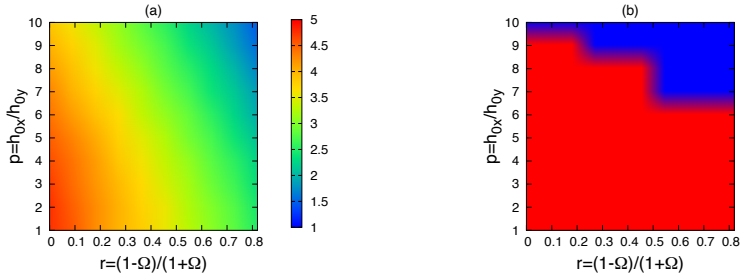

Figure 8: (a) The comprehensive phase diagram in $p-r$ plane where $p = \frac{h_{0x}}{h_{0y}}$ and $r = \frac{1-\Omega}{1+\Omega}$. The transition temperature is obtained from the position of peak of $Var(Q_x)$. (b) The nature (continuous/discontinuous) of the transition marked by different colors. The region marked by red color corresponds to the continuous or second order transition and the region of discontinuous or first order transition is marked by blue color.[17]

It has also been observed that the order of such a non-equilibrium phase transition depends on the values of h_{0x} and Ω. The order of the transition is shown as a separate image plot in h_{0x}-Ω plane. The red color represents the second-order (or continuous) transition region, whereas the blue color represents the first-order (or discontinuous) transition region. Interestingly, the boundary of these two colors is the tricritical line, observed in such a non-equilibrium phase transitions. The nature or order of the transition has been confirmed by the thermal variations of the fourth-order Binder Cumulant and the statistical distribution of the order parameter at the vicinity of the transition temperature.

I have also studied the influence of the single-site anisotropy (D) on the non-equilibrium behaviour of three dimensional XY model. Like in the case of bilinear exchange anisotropy, here I have also observed the partial symmetry breaking of the order parameter. The x-component of the order parameter (Q_x) gets dynamically ordered via dynamic symmetry breaking, while Q_y remains zero. Figure- represent the dependence of the transition temperature

T_c on the strength of single-site anisotropy (D) and also on the field amplitude h_{0x}. The comprehensive phase diagram is depicted in the plane formed by the anisotropy (D) and $p(=\frac{h_{0x}}{h_{0y}})$. The critical temperature T_c increases with an increase in anisotropy strength D for fixed value of h_{0x} (or$p$). On the other hand, the critical temperature decreases with the increase of field amplitude h_{0x}. According to the values of field amplitude (h_{0x}) and anisotropy strength (D), here also I have observed the appearance of two types of phase transition (Figure-). When the field amplitude is low, the order-disorder transition are accessed by the second-order (or continuous) transition (red region).

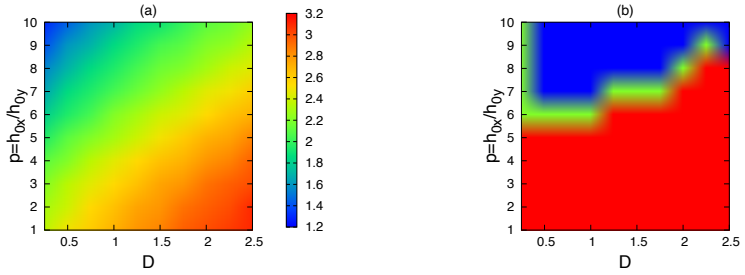

Figure 9: (a) The comprenesive phase diagram in D-p plane. The transition temperature is obtained from the position of the peak of $Var(Q_x)$. (b) The nature (continuous/ discontinuous) or order (first/second) of the transitions marked by different colors. Red: second-order, blue:first-order and green: weakly first-order region. [17]

For higher field amplitudes, such non-equilibrium transition becomes first-order (or discontinuous). The nature of transition is confirmed by the thermal variation of fourth-order Binder cumulant and the statistical distribution of order-parameter near transition region. Interestingly, for single-site anisotropy (D type), between these two regions, an additional narrow region emerges , where the amounts of discontinuity of the order parameter and the energy density are not so prominent. The energy gap during the order-disorder transition becomes smaller. It may be termed as, weakly first order region (marked by green region in Figure-9).

3 Conclusions

The study of phase transitions and critical phenomena in classical XY ferromagnets, especially under the influence of anisotropy and disorder, provides profound insights into the fundamental aspects of statistical and condensed matter physics. This thesis has comprehensively explored the equilibrium and non-equilibrium behaviors of three-dimensional anisotropic XY ferromagnets using extensive Monte Carlo simulations. The investigations have addressed the impact of constant and random anisotropy, non-magnetic impurities, quenched random fields and external elliptically polarized magnetic fields on the phase transitions and critical properties of these systems. I have focused on the equilibrium phase transitions in three-dimensional anisotropic XY ferromagnets. The systematic Monte Carlo study revealed that anisotropy breaks the inherent SO(2) symmetry of the isotropic XY model, which is crucial for the emergence of vortex-antivortex pairs and the associated Kosterlitz-Thouless transition in two dimensions. In three dimensions, this symmetry breaking leads to the destruction of vortices and the formation of long-range ferromagnetic order. The study demonstrated that the presence of constant anisotropy shifts the ferro-para phase transition to higher temperatures compared to the isotropic case. The increase in pseudocritical temperature with anisotropy strength was attributed to the enhanced ordering bias, requiring more thermal energy to disrupt the ordered phase. In contrast, random anisotropy, with its various statistical distributions, resulted in the system ordering at lower temperatures, acting as a disordering field that reduces the pseudocritical temperature. The critical exponents and phase boundaries were determined, indicating that anisotropic XY ferromagnets belong to different universality classes than their isotropic counterparts.

I have studied anisotropic XY ferromagnets with non-magnetic impurities. The presence of impurities was found to lower the critical temperature, with the decrease being proportional to the impurity concentration. The study highlighted that bilinear exchange anisotropy caused the critical temperature to increase linearly with anisotropy strength, but the rate of increase diminished with higher impurity concentrations. For single-site anisotropy,

the critical temperature decreased linearly with impurity concentration at a fixed anisotropy strength. These findings elucidate the interplay between anisotropy and impurities, showing how impurities disrupt the ordering and shift the critical behaviour.

I have studied the equilibrium behaviour of anisotropic XY ferromagnet in presence of quenched random field. The increase in critical temperature (ferro-para transition) has been noticed with increasing the strength of anisotropy. The effects of random fields (both with full circular symmetry and in angular window) on the critical temperature are investigated systematically in the anisotropic XY ferromagnet in three dimensions. Reduction of the critical temperature of anisotropic XY ferromagnet has been observed in the presence of random field. The compensating field (the required amount of field which preserves the critical temperature for isotropic XY ferromagnet) has been studied as a function of the strength of anisotropy. The compensating field was found to depend linearly on the strength of anisotropy. I have also studied the effects of random field confined in the angular window and observed the reduction of the critical temperature with increase of the angular extension. The critical behaviours are formalized by the usual finite size analysis and the estimation of critical exponents for the susceptibility and the specific heat.

Finally, I have delved into the non-equilibrium phase transitions in anisotropic XY ferromagnets subjected to elliptically polarized propagating magnetic fields. This dynamic study revealed that the system exhibits a pseudocritical temperature dependent on both the anisotropy strength and field amplitudes. The phase transitions were found to be discontinuous (first-order) for higher field amplitudes and continuous (second-order) for lower amplitudes, indicating *nonequilibrium tricritical* behaviour. The thermal variations of the order parameter's statistical distribution and the Binder cumulant confirmed the nature of these transitions. The phase diagrams illustrated the complex interplay between field strength and anisotropy, contributing to the understanding of nonequilibrium dynamics in driven systems.

I belive the research presented in this thesis is a significant contribution to the understanding of phase transitions and critical phenomena in anisotropic

XY ferromagnets, both in equilibrium and nonequilibrium conditions. The findings underscore the critical role of anisotropy and disorder in shaping the phase behavior and universality classes of these systems. The systematic Monte Carlo simulations have provided detailed phase diagrams, critical exponents, and insights into the mechanisms driving these transitions.

These investigations show the direction of further studies of equilibrium and nonequilibrium phase transitions in continuous symmetric spin models, like, Heisenberg model, XXZ, models etc. The effects of random disorder may also be studied in the case of quantum phase transitions.

In conclusion, this thesis has laid a comprehensive foundation for the study of anisotropic XY ferromagnets, highlighting the nuanced effects of anisotropy, disorder, and external fields on their critical behavior. The research outcomes not only deepen the theoretical understanding of these systems but also pave the way for future explorations into related phenomena in complex condensed matter systems.

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5 List of my Publications/ Preprints

1. Monte Carlo study of the phase transitions in the classical XY ferromagnets with random anisotropy. O. Mallick, M. Acharyya. Phase Transitions (Taylor and Francis), 96 (2023) 668-686.
   https://doi.org/10.1080/01411594.2023.2246623

2. Effects of geometry, boundary condition and dynamical rules on the magnetic relaxation of Ising ferromagnet. I. Tikader, O. Mallick, M. Acharyya. Int. J. Mod. Phys. C 34 (2023) 2350147[1] .
   https://doi.org/10.1142/S0129183123501474

3. Equilibrium and Nonequilibrium Phase transitions in continuous symmetric classical ferromagnets, O. Mallick and M. Acharyya, Invited review article published in Comprehensive Materials Processing (Elsevier) 2E, Vol-4, (2024) Pages 489-507.
   https://doi.org/10.1016/B978-0-323-96020-5.00157-6

4. Phase transitions in the anisotropic XY ferromagnet with quenched nonmagnetic impurity. O. Mallick, M. Acharyya. International Journal of Modern Physics C, 2024,2450097.
   https://doi.org/10.1142/S0129183124500979

5. Critical behaviours of anisotropic XY ferromagnet in the presence of random field. O. Mallick, M. Acharyya. J. Magn. Magn.Mater. 599(2024) 172084.
   https://doi.org/10.1016/j.jmmm.2024.172084

6. Non-equilibrium tricritical behaviour in anisotropic XY ferromagnet driven by elliptically polarised propagating magnetic field wave. O. Mallick and M. Acharyya, revised manuscript submitted in Physica A (under review).
   https://arxiv.org/abs/2403.10975

[1] not included in thesis

6 Conferences participated

1. Poster Presentation, Indian Statistical Physics Community Meeting, International Center for Theoretical Sciences, Bangalore, India, April 2024.

2. Oral Presentation, STATPHYS Kolkata XII, December 2023.

3. Poster Presentation, Indian Statistical Physics Community Meeting, International Center for Theoretical Sciences, Bangalore, India, February 2023.

4. Poster Presentation, ICCMSP, Presidency University, Kolkata, May 2022.

5. Poster Presentation, International Conference on Statistical and Computational Physics, University of Gour Banga, Malda, India, March 2022.

6. Summer school on "Nonlinear Physics and Statistical Physics", IIT Kharagpur, July 2022.

Muktish Acharyya
14.11.2024

Professor of Physics
Presidency University, Kolkata